

The theoretical and experimental investigation of the halocyclenes' phosphorylation

Cherkasov R., Galkin V., Chmutova G., Polezhaeva N., Kalinina I., Pudovik A.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The phosphorylation reactions of the oxygen- and nitrogen-containing halocyclenes - 3,4-dichloro-5-hydroxyfuranone, 3,4-dichloro-5-substituted pyrrolinon-2-ones and N-phenyl-4,5-dichloropyridazin-2-one by σ^3 -phosphorus compounds - trialkylphosphites, triphenylphosphine, and some P-functionalized derivatives of the trivalent phosphorus are studied. The reactions' mechanisms are discussed; the possible and preferable reactions' routes and the relative thermodynamic stabilities of the products and intermediates are estimated via the quantum-chemical methods.

<http://dx.doi.org/10.1080/10426500212252>

Keywords

σ^3 -phosphorus derivatives, Arbusov reaction, Halocyclenes, Phosphorylation, Quantum-chemical calculations, Reaction mechanism